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Theoretical study of the positron surface state at an alkali-metal surface

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Abstract

We present a quantum mechanical analysis of positrons trapped in a bound state at the (100) surface of bulk Cs, based on the treatment of a positron as a single charged particle trapped in an image potential-correlation well in the proximity of the surface atoms. The image-potential-induced positron surface state is calculated using the corrugated-mirror model in full three-dimensional geometry. Calculations show that the positron bound state is delocalized in the surface plane, but is strongly localized perpendicular to the surface mainly in the region between the top and the second layers of Cs atoms. The positron binding energy E_b in the surface state is computed to be 4.92 eV. Calculations on the positron annihilation rates for different Cs core levels are performed using the independent particle model. The positron surface state lifetime is calculated using the local density approximation method. The annihilation probabilities of a positron trapped at the Cs(100) surface with Cs 4p and 4d core electron levels are computed to be 0.065% and 0.22%, respectively.

1. Introduction

The long-range interaction of positrons with metal surfaces may in some cases lead to a bound state localized at the vacuum–medium interface [1]. These image-potential-induced surface states are the result of the interplay between repulsion from the surface ionic cores and the attractive electron–positron interactions and correlations just outside the surface. The existence of such positron surface states has been demonstrated by the observation that positrons could be thermally desorbed from metal surfaces at elevated temperatures as positronium [2]. Recently positron surface states have become the subject of experimental studies using positron-annihilation-induced Auger electron spectroscopy (PAES), which employs positrons trapped at the surface to annihilate with the neighboring core-level electrons [3]. This new technique provides an experimental tool to make site-sensitive studies of the positron annihilation process, and motivated this work.

In this paper we present a first-principles study of the positron bound state at a Cs(100) surface. The trapping of positrons at a surface is described on the basis of a simple long-range image potential, truncated at the surface. The three-dimensional potential due to the Cs(100) surface is constructed using the corrugated mirror model [4], which matches a local

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